**Relativistic Quantum Mechanics**

As we know, any theory must be compatible with Einstein’s theory of special relativity. This was recognized by Schrodinger and Heisenberg, etc., when they were trying to develop quantum mechanics, and they attempted from the first to make it fully compatible with special relativity. But they were unsuccessful with this, and only later realized that their formulations of quantum mechanics were none-the-less quite accurate in non-relativistic domains. It remained for Paul Dirac to develop a satisfactory relativistic formulation three years later in 1929. The usefulness of the Dirac equation is that it:

(1) predicts the spin states of the electron from first principles (so far we’ve had to add the spin degrees of freedom to the Hilbert space ad hoc),

(2) it predicts the (almost correct value of the) anomalous g-factor moreover appearing in the Hamiltonian for a spin in a magnetic field,

(3) and it correctly predicts the fine-structure corrections to the Hydrogen energy spectrum.

It also has some issues though, which we’ll get to in time.

**Criteria for relativistic ‘Schrodinger’ equation**

This is what we want out of any relativistic ‘Schrodinger’ equation. For one, we want it to be relativistically invariant, meaning when we make a Lorentz change of variables, the equation is invariant. And secondly we want the equation to naturally incorporate a particle’s spin degrees of freedom into the equation, and we’d also like an equation which predicts the anomalous g-factor appearing in the electron’s magnetic moment. We’ll explore these two a little more below.

**Relativistic invariance**

We need Lorentz invariance because according to Einstein, the laws of physics are invariant with respect to any inertial frame. The Schrodinger equation as presently written is not invariant. For example, let’s take a look at the free-particle Schrodinger equation in 1D (in position space)



Now let’s make a Lorentz change of variables to a primed reference frame moving at speed v to the right. The coordinates in the primed frame are related to the stationary frame coordinates by:





So filling these in we have the Schrodinger equation in the primed coordinates to be:



which is not the same equation by any stretch, though we will note that it is in the case where β → 0 and γ → 1 which is the classical limit. So why does it fail? Basically because the Schrodinger equation treats the time and position variables differently. The equation is first order in t and second order in x. So in order to make the equation relativistically invariant we will need an equation which treats both variables to the same order.

**Incorporation of spin d.o.f.**

Secondly we want the equation to naturally incorporate spin degrees of freedom instead of making us include it ad hoc as we’ve done so far. Mathematically, this means that we would like the relativistic ‘Schrodinger’ equation to be a 2 component matrix equation. And hopefully, when we incorporate the magnetic field into the equation, the g-factor will come out naturally.

**Klein-Gordon Equation**

Let’s go back to the Schrodinger equation – free particle for now,



So far we have been using the classical expression for the energy of a particle. Perhaps if we use instead the actual relativistic expression for the energy we’ll have our desired equation. So we would write,



This looks promising perhaps, but it still wouldn’t be relativistically invariant, as we can tell when we write it in position space,



because it still treats **r** and t at different orders. Plus, I’m not sure how mathematically well defined the √operator is. One possibility is to square both sides of the equation. When we do we get the so-called Klein-Gordon equation:



If we put this into position space, we’ll have:



which we can write as:



If we use the metric ημν = (+1, -1, -1, -1), as is convention in relativistic quantum mechanics/quantum field theory, then we may write this as:



Where we recognize ∂2 as the wave-operator, box, or whatever you want to call it, and as the magnitude of the SR gradient (see Special Relativity tensor stuff in Classical Mechanics):



Since,



As a scalar, it is invariant, and so the KG equation is relativistically invariant as required.

So that’s good, but there is a major problem. Consider our interpretation of the wavefunction. We normally would say that ρ = ψ\*ψ, and **j** = Re(ψ\*ψ). However we identify ρ and **j**, they must be related via the continuity equation:



But if we define ρ as ψ\*ψ, one can see that we won’t be able to satisfy this form. Instead, we can define:



Then consider the time derivative,



We can fill in the KG equation,



and so identify:



The ρ is unlike what we’re accustomed to, though **j** is familiar. But the problem here is that there is no guarantee that ρ will actually be positive, thanks to the minus sign. And so it cannot be interpreted as a probability density. This was deemed a fatal flaw, though it turns out the equation still finds use in QFT. Another problem though is that it doesn’t force a two – component matrix representation of a particle upon us. As a consequence, the equation cannot describe a spin-full particle. It would be restricted to describing spin-0 bosons, which it does quite well in QFT context. But its not what we want since we want to be able to describe fermions.

**Dirac Equation**

So go back to:



If we could somehow write the term inside the √ as a perfect square, then we could have an equation first order in t and **r** and so would also be relativistically invariant. So we would want to determine numbers **α** (**α** is a vector in fact) and β such that:



What are the properties of **α** and β that could make this possible? Let’s work it out…



where we’re using the standard notation:



Thus we see that for both sides to be equal, we must have:



which implies that these ‘numbers’ αi and β *cannot* be numbers! For instance, consider the first requirement. It implies that α1α2 + α2α1 = 0. But if these were numbers then that would imply that either α1 or α2 must be zero. But we also need {α1,α1} = 2, and {α2,α2} = 2 → neither α1 nor α2 can be zero. So clearly ordinary numbers do not satisfy these properties, and nor did we expect them to. The resolution to this dilemma is that the entities **α** and β must be *operators* (*or matrices in other words*). And this is actually encouraging because we wanted a matrix Schrodinger equation to develop in the first place. So what are these matrices, **α** and β? The anti-commutation relations alone are not enough to completely specify them. In fact, any unitary transformation **α** → U**α**U-1 and β → UβU-1 will also satisfy these commutation relations. Nonetheless we can develop a representation of these matrices. First let’s consider a few properties:

**α and β are Hermitian**

We demand that αi and β are Hermitian matrices because we need the Hamiltonian to be Hermitian.



**α and β are traceless**

We can prove the matrices are traceless as follows. Consider αi for example. We have from the anti-commutation relation:



but we can also say, using the anti-commutation relations that:



And so we have that Tr(αi) = - Tr(αi) which implies that it is zero. We can make the same argument with β to conclude:



**α and β have eigenvalues of 1 or -1**

Let |a> be an eigenvector of αi with eigenvalue a. Since we have:



it follows that:



We can make the same argument with β. So we have:



**α and β must be even-dimensional matrices**

This follows from the following consideration. Let U be the unitary matrix of orthonormal eigenvectors of αi or β. Then Ai = UαiU-1, or B = UβU-1 will be the diagonal matrix of eigenvalues of αi or β respectively. Then consider:



where m is the number of 1 eigenvalues of αi, and n is the number of -1 eigenvalues of αi. Now also know that Tr(αi) = 0 from above. So m must be equal to n. Now the number of eigenvalues D = m + n is just the dimensionality of the matrix, and so if m = n, then D = 2m = even number. So the dimensionality of the matrix is even. Repeating the argument for β we have:



**Determining the representation of the matrices α and β**

Now we want to use this information to help us determine what these matrices are. The anti-commutation relation should be familiar to us as identical to that of the spin matrices. So perhaps we could identify where



? Then what would β be? Let’s assume some form that is Hermitian and traceless:



where β11 is real. And now let’s impose the condition that its square be 1.



which implies that:



and now impose the anti-commutation relation with say α1. Then we must have:



So we find that β12­ must be imaginary. So let’s write it as β12 = ib. Now let’s do the anti-commutation relation with α2,



which implies that b = 0. So β12 = 0. But then β11 = 0 by the first condition. So all the elements of β are 0. But this cannot satisfy the anti-commutation relations. So in fact there is no β that can satisfy these relations. So we have to go to 4D. It *is* possible to find a representation in 4D. And after playing around a bit, one representation we’d find is:



or explicitly,



another representation is the Weyl representation:



And with these matrices, we can write down the so-called Dirac equation which is the relativistic generalization of the Schrodinger equation for spin ½ particles,



Finally, if we want to include a potential we would write,



Be sure to note that the matrices **α** and β are to be interpreted as *operators* in the (Lorentz) spinor space of the fermion – that’s why I’ve put carrots on top of them. They are the relativistic generalizations of the Pauli spin matrices, **σ**, which are themselves operators in the spin space of the fermion in the non-relativistic theory given by the Schrodinger equation. These operators have particular representations if we go to (Lorentz) spin space and these representations are given by the matrices above. Of course **α** and β are 4D matrices, and not 2D matrices, unlike **σ**, so now ψ is a 4-component object instead of 2. It is called a Lorentz spinor. We are a little perplexed at this 4 dimensionality now, but we will see how to interpret this in a bit. Let’s look at a few cases.

Before quitting, I guess I’ll throw in that it is conventional to write the free, position space version differently. We define matrices:



which in the Dirac representation reduce to:



and in the Weyl representation, to:



then, multiplying both sides of our equation by β (and noting β2 = 1), we have:



In units whereby ℏ = 1, c = 1, this reduces to (leaving ψ as |ψ> because we haven’t projected onto spinor space and so its still a ket in that sense):



where ∂μ = (∂t, ∂x, ∂y, ∂z). Now it’s convention to define the notation:



And so we can write this as:



Now let’s revisit the interpretation of the wavefunction issue. For the sake of discussion, we’ll presume/hope that we still have ρ = ψ†ψ so that the density is guaranteed to be positive definite. And let’s look at the derivatives of |ψ> and <ψ|, in position space (again, keeping the |> because its still a spinor in spinor space):



and then taking the dagger of both sides, and using the Hermiticity of those operators:



The arrows are to indicate which direction the operators are operating. It’s kind of obvious right now, but in a second….so let’s take the derivative of our prospective density:



Note we are able to take the arrows off of α because its Hermiticity allows it to act in any direction. Comparing with the continuity equation, we see that we have:



which is definitely unintuitive apropos the current density, but the important thing is that we have a continuity equation with a ρ which we can interpret as a probability density. We can put this in terms the γ matrices.



Define the ‘Hermitian adjoint’ as:

,

and we can say:



and in general we can define a 4-current:



in terms of which the continuity equation takes a covariant form:



This really will be relativistically covariant, and the Dirac equation too, as long as γμ transforms as a tensor under a Lorentz transformation. We’ll investigate this stuff next file.

**Hilbert Space**

So now our wavefunction exists in an enlarged HS:



where ms spans 4 dimensional column vector space (spinor space), instead of the previous 2 dimensional space it used to reside in. So we can say,



We’ll typically just write this as:



where **χ** and **Φ** are both 2D column vectors. And we’ll notate:



for short. This notation is handy because the Dirac equation is block diagonal/off diagonal, and so doesn’t split up the components of **χ** and **Φ**. A general wavefunction will now look like,



**Representation of Observables**

So the usual real space observables like r, p, L, H, etc. don’t change. And they would just be written as usual, multiplied by a 4D unit matrix in our augmented HS. The spin operator already operates in half the space, and now we’d just carry it over to the other half. We’d say:



where **σ** is the 2D vector Pauli-spin matrix. As noted above, we have two new operators , and . And their explicit representation in this 4D space is:



These are Hermitian. I wonder if they correspond to any particular observable? And we have the related γ operators,



**Time-Development**

We must still have:



**Some nice operator identities**

Before stopping for the moment, let’s consider a useful identity. Let M and N be vector operators. Then consider the following construction:



So,



And consequently



or for short, leaving out the implicit identity matrix,



Note it follows in particular that:



Can also go to higher order products,



Then use,



to write,



And so we have:



And with that formula, we could continue to reduce any product of σ’s back down to some linear combination. The γμ also have worthwhile properties to investigate. Consider the Weyl representation. It’s often written in shorthand as:



where **1** is the identity matrix, not a vector. Might note that:



and in particular,



Now let’s look at anti/commutation relations. First the Dirac representation:



and also have:



The anticommutation relations are generally written succinctly as:



Apropos the Weyl representation we have:



and also have:



And we can say, like before,



All the relations are the same, w/r to themselves, as we’d expect since they’re related via unitary transformation. Here’s some more:



and being overly meticulous,



which implies,



where **1** is a 4×4 identity matrix. Now just want to look at the rotation matrix, in spin basis. First, using:



we have that:



etc., and so:



and we get:



This sort of construction will be useful when we consider Lorentz boosts to spinors.